

Materials with a desired refraction coefficient can be made by embedding small particles.

A. G. Ramm

(Mathematics Department, Kansas St. University,
Manhattan, KS66506, USA
and TU Darmstadt, Germany)
ramm@math.ksu.edu

Abstract

A method is proposed to create materials with a desired refraction coefficient, possibly negative one. The method consists of embedding into a given material small particles. Given $n_0(x)$, the refraction coefficient of the original material in a bounded domain $D \subset \mathbb{R}^3$, and a desired refraction coefficient $n(x)$, one calculates the number $N(x)$ of small particles, to be embedded in D around a point $x \in D$ per unit volume of D , in order that the resulting new material has refraction coefficient $n(x)$.

PACS: 03.04.Kf

MSC: 35J05, 35J10, 70F10, 74J25, 81U40, 81V05

Keywords: "smart" materials, wave scattering by small bodies, many-body scattering problem, negative refraction, nanotechnology

1 Introduction

There is a growing interest to materials with the desired properties, in particular, with negative refraction coefficient (see [1] and references therein). In [2] the role of spatial dispersions is emphasized in explaining unusual properties of materials. In [3] the role of dispersion for wave propagation in solids is described. In [4] boundary-value problems in domains with complicated boundaries were studied. In [6], [7] wave scattering by small bodies of arbitrary shapes is studied and formulas for the S -matrix are obtained. In [5] a general method for creating materials with wave-focusing properties is proposed and justified. Our aim in this paper is to use a similar approach for creation of the materials with a desired refraction coefficient by embedding small particles into a given material with

known refraction coefficient $n_0(x)$. The acoustic wave scattering by the given material is described by the Helmholtz equation

$$[\nabla^2 + k^2 n_0(x)]u = 0 \text{ in } \mathbb{R}^3, \quad n_0(x) = \begin{cases} 1 & \text{in } D' := \mathbb{R}^3 \setminus D, \\ n_0(x) & \text{in } D. \end{cases} \quad (1)$$

Here $k > 0$ is the wavenumber in D' . Equation (1) can be written as the Schrödinger equation

$$L_0 u := [\nabla^2 + k^2 - q_0(x)]u = 0 \text{ in } \mathbb{R}^3, \quad q_0 := k^2 - k^2 n_0(x). \quad (2)$$

We assume $k > 0$ fixed and do not show k -variable in q_0 . Clearly, $q_0 = 0$ in D' . The scattering solution to (2) is uniquely defined by the radiation condition:

$$u_0 = e^{ik\alpha \cdot x} + A_0(\beta, \alpha) \frac{e^{ikr}}{r} + o\left(\frac{1}{r}\right), \quad r := |x| \rightarrow \infty, \quad \beta := \frac{x}{r}. \quad (3)$$

Here $\alpha \in S^2$ is a given unit vector: the direction of the incident plane wave, S^2 is the unit sphere in \mathbb{R}^3 , $A_0(\beta, \alpha)$ is the scattering amplitude, and β is the unit vector in the direction of the scattered wave.

Assume that M small particles D_m , $1 \leq m \leq M$, are embedded into D . Smallness means $n_0 k a \ll 1$, where $a = 0.5 \max_m \text{diam } D_m$, and $n_0 = \max_{x \in D} |n_0(x)|$. On the boundary S_m of D_m an impedance boundary condition is satisfied:

$$u_N(s) = \zeta_m u(s), \quad s \in S_m, \quad 1 \leq m \leq M,$$

where N is the unit normal to S_m pointing out of D_m . We assume that the surface S_m is Lipschitz, and the Lipschitz constant does not depend on m , $1 \leq m \leq M$. The scattering problem can now be stated as follows:

$$L_0 u = 0 \text{ in } \mathbb{R}^3 \setminus \bigcup_{m=1}^M D_m, \quad u_N = \zeta_m u \text{ on } S_m, \quad 1 \leq m \leq M, \quad (4)$$

$$u(x) = u_0(x) + A_M(\beta, \alpha) \frac{e^{ikr}}{r} + o\left(\frac{1}{r}\right), \quad r = |x| \rightarrow \infty, \quad \beta = \frac{x}{r}. \quad (5)$$

We prove that the solution to problem (4) – (5) converges as $M \rightarrow \infty$ to the solution of the problem

$$L\mathcal{U} := [\nabla^2 + k^2 - q(x)]\mathcal{U} = 0 \text{ in } \mathbb{R}^3, \quad (6)$$

$$\mathcal{U} = e^{ik\alpha \cdot x} + A(\beta, \alpha) \frac{e^{ikr}}{r} + o\left(\frac{1}{r}\right), \quad r = |x| \rightarrow \infty, \quad \beta = \frac{x}{r}, \quad (7)$$

where

$$q(x) = q_0(x) + p(x), \quad (8)$$

and give a formula for $p(x)$. It turns out that $p(x)$ can be made an arbitrary desired function by choosing the density of the number $N(x)$ of the embedded particles around each point $x \in D$ and the impedances ζ_m properly. Thus, $q(x)$ can be made an arbitrary desired function. Therefore the refraction coefficient

$$n(x) = 1 - k^{-2}q(x) = n_0(x) - k^{-2}p(x) \quad (9)$$

can be made arbitrary, in particular, negative.

If $n_0(x)$ is given and one wishes to create the material with the coefficient $n(x)$, then one calculates

$$p(x) = [n_0(x) - n(x)]k^2,$$

and embeds $N(x)$ small particles per unit volume of D around each point $x \in D$ and chooses their impedances ζ_m so that the function $p(x)$ is obtained for the new material. In Section 2 we give analytical formulas for $N(x)$ and ζ_m and sufficient conditions for the convergence of the solution to (4) – (5) to the solution of (6) – (8) as $M \rightarrow \infty$ in such a way that relations (13)-(14) hold.

We also prove that the relative volume of the embedded particles is negligible. More precisely, if $|D_m|$ the volume of D_m , then

$$\lim_{M \rightarrow \infty} \frac{\sum_{m=1}^M |D_m|}{D} = 0.$$

By $|S_m|$ we denote the surface area of S_m . We use an approximate formula for the electric capacitance of the perfect conductor with boundary S (see [6], p.26, formula (3.12)):

$$C_m^{(0)} \approx \frac{4\pi|S_m|^2}{J_m}, \quad J_m := \int_{S_m} \int_{S_m} \frac{ds dt}{|s - t|}. \quad (10)$$

Note that

$$C_m^{(0)} = O(a), \quad |S_m| = O(a^2), \quad J_m = O(a^3).$$

By $C_m^{(0)}$ the electric capacitance of a perfect conductor with the surface S_m is denoted. We assume that

$$n_0 k a \ll 1, \quad d \gg a, \quad d := \min_{m \neq j} \text{dist}(D_m, D_j). \quad (11)$$

Let

$$C_{m\zeta_m} := C_m^{(0)} [1 + C_m^{(0)} (\zeta_m |S_m|)^{-1}]^{-1}. \quad (12)$$

We assume throughout the paper that

$$d = O(a^{1/3}), \quad a = O\left(\frac{1}{M}\right).$$

Let $M \rightarrow \infty$ and assume that the following limit exists:

$$\lim_{\substack{M \rightarrow \infty \\ |x_m - x| \leq d}} C_m^{(0)}(\zeta_m |S_m|)^{-1} := h(x). \quad (13)$$

Here and below $x_m \in D_m$ is an arbitrary point in D_m . Because D_m is small, the choice of this point in D_m is not important. Under the assumed relations between a and d one has $\lim_{M \rightarrow \infty} \frac{a}{d} = 0$. The limit (13) exists if and only if $\zeta_m = O(a^{-1})$, because $|S_m| = O(a^2)$ and $C_m^{(0)} = O(a)$.

Denote by $N_m(x)$ the number of small particles per unit volume around a point $x \in D$: $\int_{\tilde{D}} N_M(x) dx = \sum_{D_m \subset \tilde{D}} 1$ for any subdomain $\tilde{D} \subset D$.

The number of particles per unit volume is $O(\frac{1}{d^3}) = O(\frac{1}{a})$. Therefore their relative volume is $O(\frac{a^3}{d^3}) = O(a^2) \rightarrow 0$ as $M \rightarrow \infty$. On the other hand, the quantity $N_M(x)C_{m\zeta_m}$, which has physical meaning of the average quantity $C_{m\zeta_m}$ per unit volume of D around point x , has a limit:

$$\lim_{\substack{M \rightarrow \infty \\ |x_m - x| \leq d}} N_M(x)C_{m\zeta_m} = \frac{C(x)}{1 + h(x)}, \quad \lim_{\substack{M \rightarrow \infty \\ |x_m - x| \leq d}} N_M(x)C_m^{(0)} := C(x). \quad (14)$$

The existence of the finite second limit in (14) is clear because $N_M(x) = O(\frac{1}{a})$ and $C_M^{(0)} = O(a)$, and the existence of the first limit in (14) follows from formula (13) and from the second formula (14). Our basic result is the formula:

$$[n_0(x) - n(x)]k^2 := p(x) = \frac{C(x)}{1 + h(x)}, \quad (15)$$

where $C(x)$ is defined in (14) and $h(x)$ is defined in (13).

Example 1. Suppose $\zeta_m = \infty$, so $\mathcal{U}|_{S_m} = 0$, which corresponds to acoustically soft particles. Then $h(x) = 0$, $p(x) = C(x)$. Assume that the small particles are balls of radius a . Then $C_m^{(0)} = a$, $N_M(x) = \frac{p(x)}{a}$, $M = O(\frac{1}{a})$. Since $N_M(x) > 0$ and $C_m^{(0)} > 0$, then $p(x) \geq 0$, so one can create in this case only non-negative functions $p(x)$. For any positive function $p(x)$ one should embed $N(x) = \frac{p(x)}{a}$ small acoustically soft balls of radius a per unit volume of D around each point $x \in D$, and the resulting material will have $n(x) = n_0(x) - k^{-2}p(x)$. In particular, $n(x) < 0$ if $p(x) > k^2 n_0(x)$.

Example 2. Choose an arbitrary function $p(x) = p_1(x) + ip_2(x)$, $p_2(x) \leq 0$. The condition $p_2 \leq 0$ guarantees uniqueness of the solution to problem (6)-(7) with $q(x) = q_0(x) + p(x)$. Physically this condition means that the medium, corresponding to $n(x) = 1 - k^{-2}q(x)$ has nonnegative absorption. Let the particles be balls of radius a and $\zeta_m = \zeta_m(x) = \frac{1}{4\pi a h(x)}$, where $h(x)$ is an arbitrary function at the moment. This function is fixed later. Then formula (13) holds because

$|S_m| = 4\pi a^2$. Choose $N = N(x)$ and $h(x) = h_1 + ih_2$ from the first equation (14) using (12):

$$p_1 + p_2 = \frac{Na}{1 + h(x)} = \frac{Na(1 + h_1 - ih_2)}{(1 + h_1)^2 + h_2^2}.$$

Thus,

$$p_1 = \frac{Na(1 + h_1)}{(1 + h_1)^2 + h_2^2}, \quad p_2 = -\frac{Nah_2}{(1 + h_1)^2 + h_2^2}. \quad (16)$$

We have three functions: $N = N(x) > 0$, h_1 and h_2 , to satisfy two equations (16). This can be done by infinitely many ways. For instance, one can take $h_1 = 0$, $h_2 = -\frac{p_2}{p_1}$ and $N = a^{-1}p_1(1 + \frac{p_2^2}{p_1^2})$. Thus, to get the material with the desired $n(x) = n_0(x) - k^{-2}p(x)$, where $p(x) = p_1(x) + ip_2(x)$, one embeds $N(x) = a^{-1}(p_1^2 + p_2^2)/p_1$ small balls of radius a per unit volume around each point x and chooses the impedance $\zeta_m(x) = (4\pi ah(x))^{-1}$, where $h = h_1 + ih_2$, $h_2 = -p_2/p_1$, $h_1 = 0$.

2 Derivation of the results.

We seek the unique solution to (4) – (5) of the form

$$\begin{aligned} u &= u_0 + \sum_{m=1}^M \int_{S_m} G(x, t) \sigma_m(t) dt \\ &= u_0 + \sum_{m=1}^M G(x, x_m) Q_m + \sum_{m=1}^M \int_{S_m} [G(x, t) - G(x, x_m)] \sigma_m dt. \end{aligned} \quad (17)$$

Here $L_0 G_1 = \delta(x - y)$ in \mathbb{R}^3 , G satisfies the radiation condition, σ_m are to be chosen so that the boundary condition (4) is satisfied, $Q_m := \int_{S_m} \sigma_m dt$, $x_m \in D_m$. In the generic case $Q_m \neq 0$ one can neglect the last term in (17) compared with the preceding term if $|x - x_m| > d \gg a$ for all m . Indeed, under this assumption one has $|G(x, t) - G(x, x_m)| \leq |\nabla_y G(x, \tilde{y}) \cdot (t - x_m)| = O(\frac{a}{d}) \ll 1$, where $\tilde{y} := x_m + \tau(t - x_m)$, $0 < \tau < 1$, is a 'middle point'. Thus, the third term on the right side of (17) is $O(\frac{a}{d} |Q_m|) \ll |Q_m|$, where we also assume that $|Q_m| = O(\int_{S_m} |\sigma_m| dt)$. We will see that this assumption is justified. For example, if $u|_{S_m} = 0$, then σ_m does not change sign on S_m . Thus, generically one can write

$$u = u_0(x) + \sum_{m=1}^M G(x, x_m) Q_m, \quad |x - x_m| \geq d \gg a, \quad (18)$$

with the error $O(\frac{a}{d})$. The choice of $x_m \in D_m$ does not matter because a is small. One may assume that D_m are convex and take x_m at the gravity center of D_m .

The functions $G(x, y)$ and $u_0(x)$ are known because $n_0(x)$ is known. Let us derive an equation for finding Q_m . If Q_m are found then the scattering problem (4) – (5) is solved by formula (18) for any x away from an immediate neighborhood of the small particles. To derive an equation for Q_m we need some preparations. The function $G(x, y)$ solves the equation:

$$G(x, y) = g(x, y) - \int_D g(x, z)q(z) G(z, y)dz, \quad g(x, y) := \frac{e^{ik|x-y|}}{4\pi|x-y|}. \quad (19)$$

One can easily prove that

$$G(x, y) = g(x, y)[1 + O(|x - y|)] = g_0(x, y)[1 + O(|x - y|)], \quad |x - y| \rightarrow 0, \quad (20)$$

where $g_0(x, y) = (4\pi|x - y|)^{-1}$. Let

$$T_j\sigma_j := \int_{S_j} G(s, t) \sigma_j(t)dt, \quad A_j\sigma_j = 2 \int_{S_j} \frac{\partial g_0(s, t)}{\partial N_s} \sigma_j(t)dt. \quad (21)$$

It is known ([6], p. 91) that

$$\int_{S_j} A_j\sigma_j dt = - \int_{S_j} \sigma_j(t)dt, \quad \frac{\partial(T_j\sigma_j)}{\partial N_s} = \frac{A_j(k)\sigma_j - \sigma_j}{2}, \quad (22)$$

where $A_j(k)$ is the operator similar to (21) with $g(s, t)$ in place of $g_0(s, t)$, $N_s := N$ is the outer normal to S_j at the point $s \in S_j$. On the surface S_j we have

$$u = u_e(s) + T_j\sigma_j, \quad u_e := u_0 + \sum_{m \neq j}^M G(s, x_m)Q_m. \quad (23)$$

Using boundary condition (4) and formulas (22), (23), one gets

$$u_{e_N}(s) - \zeta_j u_e(s) + \frac{A_j\sigma_j - \sigma_j}{2} - \zeta_j T_j\sigma_j = 0. \quad (24)$$

Integrate (24) over S_j , use (22) and get:

$$Q_j = \int_{S_j} u_{e_N}(s)ds - \zeta_j \int_{S_j} u_e(s)ds - \zeta_j \int_{S_j} T_j\sigma_j ds. \quad (25)$$

One has

$$\int_{S_j} u_{e_N}ds = \int_{D_j} \Delta u_e dx = O(k^2 a^3), \quad \int_{S_j} u_e ds = u_e(x_j)|S_j| = O(a^2),$$

where the smallness of D_j and the fact that u_e and its two derivatives are bounded on S_j were used. Since $ka \ll 1$ we can neglect the first integral in (25) compared with the second. Furthermore

$$I := \int_{S_j} T_j\sigma_j ds = \int_{S_j} dt\sigma_j(t) \int_{S_j} \frac{ds}{4\pi|s - t|}.$$

We replace the last integral by its mean value

$$\frac{1}{|S_j|} \int_{S_j} dt \int_{S_j} \frac{ds}{4\pi|s-t|} := \frac{J_j}{4\pi|S_j|}.$$

Thus, $I = \frac{J_j Q_j}{4\pi|S_j|}$, and (25) yields:

$$Q_j = -\frac{\zeta_j |S_j|}{1 + \zeta_j J_j (4\pi|S_j|)^{-1}} u_e(x_j). \quad (26)$$

We have replaced $u_e(s)$ by $u_e(x_j)$ because $|x_j - s| < 2a$ and a is small while $u_e(x)$ is continuous in a neighborhood of x_j . Using (10) we rewrite (26) as

$$Q_j = -C_j^{(0)} [1 + C_j^{(0)} (\zeta_j |S_j|)^{-1}]^{-1} u_e(x_j) := -C_{j\zeta_j} u_e(x_j). \quad (27)$$

Thus, (18) can be written as:

$$u(x) = u_0(x) - \sum_{m=1}^M G(x, x_m) C_{m\zeta_m} u(x_m), \quad |x - x_m| \geq d \gg a. \quad (28)$$

We have replaced $u_e(x_m)$ by $u(x_m)$ under the sign of the sum in (28) because at the points x which are away from small particles one has $u_e(x) = u(x)$ with the error $O(\frac{a}{d})$. Formulas (13) – (14) allow one to pass to the limit $M \rightarrow \infty$ in (28) and get

$$\mathcal{U}(x) = u_0(x) - \int_D G(x, y) p(y) \mathcal{U}(y) dy, \quad (29)$$

where $p(x)$ is defined in (15). Applying to (29) the operator L_0 , defined in (2), and using the relation $L_0 G(x, y) = -\delta(x - y)$ yields equation (6) with q defined in (8). The radiation condition for \mathcal{U} is satisfied:

$$A(\beta, \alpha) = A_0(\beta, \alpha) + A_1(\beta, \alpha), \quad (30)$$

where

$$A_1(\beta, \alpha) = \lim_{M \rightarrow \infty} A_M(\beta, \alpha) = -\frac{1}{4\pi} \int_D u_0(y, -\beta) p(y) \mathcal{U}(y) dy. \quad (31)$$

Here we have used a result from [8]:

$$G(x, y) = \frac{e^{ik|x|}}{4\pi|x|} u_0(y, -\beta) + o\left(\frac{1}{|x|}\right), \quad |x| \rightarrow \infty, \quad \frac{x}{|x|} = \beta. \quad (32)$$

In our derivations it was assumed that $\zeta_m \neq 0$. If $\zeta_m = 0$ for all m , that is, the small particles are acoustically hard, then $Q_m = 0$ in the first order with respect to ka . One can show that in this case $Q_m = O(k^2 a^3)$, and that the last sum

in (17) is of the same order of magnitude as the preceding sum. Consequently, the theory in this case is quite different: the effective field in the medium is not described by equation (29), which is equivalent to a local equation (6). In fact, the effective field in this case is described by an integrodifferential equation which is not equivalent to a local differential equation.

Let us explain the relation $Q_m = O(k^2 a^3)$, mentioned above. Write (24) with $\zeta_j = 0$, integrate over S_j and use the first formula (22) to get

$$Q_j = \int_{S_j} u_{e_N} ds = \int_{D_j} \Delta u_e dx = O(k^2 a^3).$$

References

- [1] Agranovich, V.M., Gartstein, Yu.N., Spatial dispersion and negative refraction of light, *Uspekhi Phys. Nauk*, 176,N10, (2006), 1051–1068.
- [2] Agranovich, V.M., Ginzburg, V.L., *Crystal optics with spatial dispersion and excitons*, Springer-Verlag, Berlin, 1984.
- [3] Landau, L.D., Lifshitz, E.M., *Electrodynamics of continuous media*, Pergamon Press, Oxford, 1984.
- [4] Marchenko, V., Khruslov, E., *Boundary-value problems in domains with fine-grained boundary*, Naukova Dumka, Kiev, 1974.
- [5] Ramm, A.G., Distribution of particles which produces a "smart" material, *Jour. Stat. Phys.*, 127, N5, (2007), 915-934.
- [6] Ramm, A.G., *Wave scattering by small bodies of arbitrary shapes*, World Sci. Publ., Singapore, 2005.
- [7] Ramm, A.G., Wave scattering by small particles in a medium, *Phys. Lett. A.*, (2007) (to appear)
- [8] Ramm, A.G., *Inverse problems*, Springer, Berlin, 2005.